Modeling Granular Particle Shape Using Discrete Element Method

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presented by

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Outline

- Background
- Research Objectives
- Data Set
- Shape Characterization
- Discrete Element Modeling
- Results
- Conclusions

Background

- Particle morphology governs micromechanical behavior of granular media
- Traditionally, 2-D analyses adopted in studying influence of particle shapes on mechanical response of cohesionless soil and most analyses are limited to circular or idealized shapes
- Limited knowledge available on 3-D discrete element modeling of highly irregular particle shape
- Discrete Element Method (DEM) can be used in modeling particle shape in two and three dimensions

Background

- Particle shape modeling techniques in 2-D using DEM
  - Circular/spherical discrete elements: Cundall and Strack (1979)
  - Polygonal discrete elements: Barbosa and Ghaboussi (1992)
  - Elliptical discrete elements: Ting et al. (1993)
  - Overlapping discrete element cluster (ODEC): Ashmawy et al. (2003)
- Particle shape modeling techniques in 3-D
  - 3-D ellipsoid-based DEM - ELLIPSE3D: Lin and Ng (1997)
  - Polyhedron-based approach: Ghaboussi and Barbosa (1990)
  - 3-D image-based DEM: Matsushima (2004)

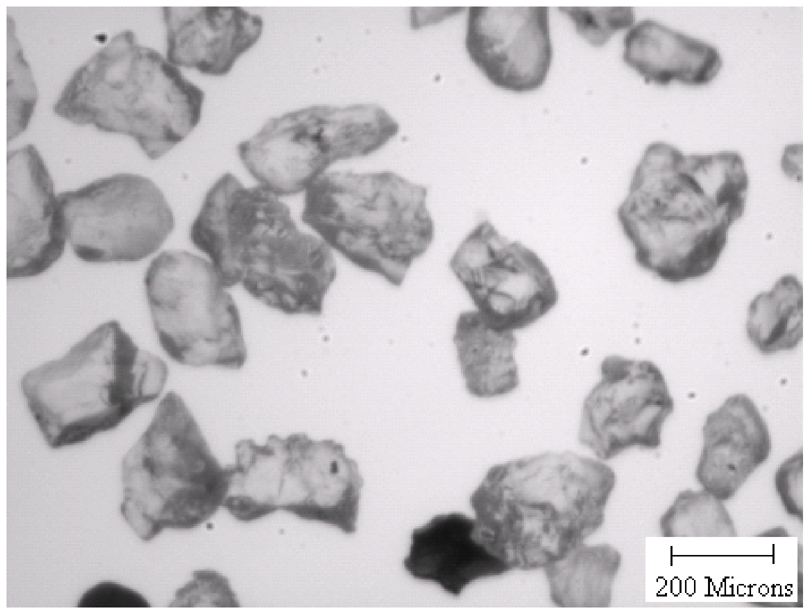
Need for Particle Shape Modeling

- DEM simulations are typically limited to circular or spherical particles for computational efficiency. As a result:
  - Particle rotation is excessive
  - Dilation is suppressed
  - Particle interlocking is reduced
- Non-circular simulations (e.g., ellipses) are unrealistic
- More complex shapes (e.g., polygons) are computationally inefficient

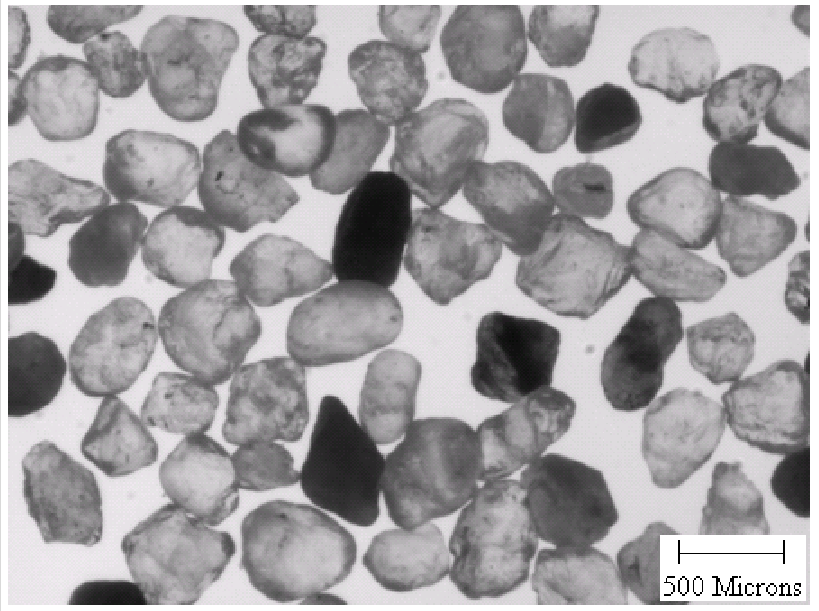
Research Objectives

- To design and develop automated 3-D tomography reconstruction algorithms applied to shape characterization of sand particles
- 2-D and 3-D discrete element modeling of particle shape
- Evaluation of influence of particle shape on shear strength of soil

Data Set



Daytona Beach Sand



Michigan Dune Sand

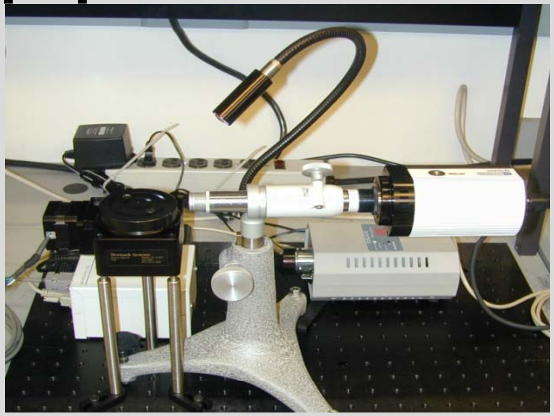
Particle Shape Characterization

Equipment used for shape characterization

2-d image capture using regular microscope

3-d image capture equipment

SkyScan X-Ray CT System



Optical Tomography System

Online database

http://www.rowan.edu/colleges/engineering/clinics/shreek

[*] = Number of Particles

- Online geomaterial database
  - Computed Tomography
    - X-ray tomography
      - Michigan Dune [8]
      - Standard Melt [7]
      - Dry #1 [6]
      - Rhode Island [7]
      - Ala Wai Beach [5]
      - Kahala Beach [7]
      - Daytona Beach [5]
    - Optical tomography
      - Michigan Dune [8]
      - Standard Melt [7]
      - Dry #1 [6]
      - Rhode Island [7]
      - Ala Wai Beach [5]
      - Kahala Beach [7]
      - Daytona Beach [5]
  - Optical Microscopy
    - Michigan Dune [293]
    - Standard Melt [391]
    - Dry #1 [382]
    - Daytona Beach [299]

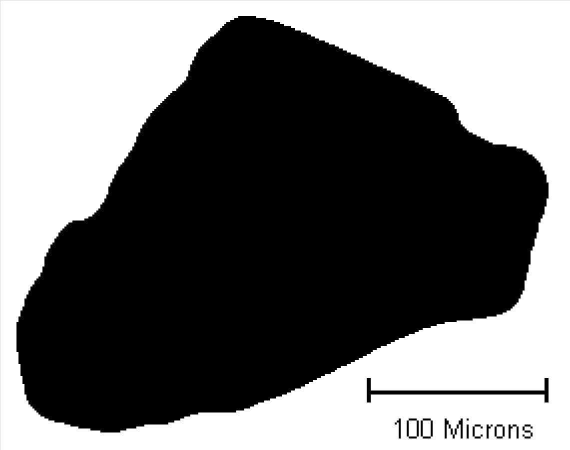
Particle Shape Modeling

Process for Modeling of Particle Shape

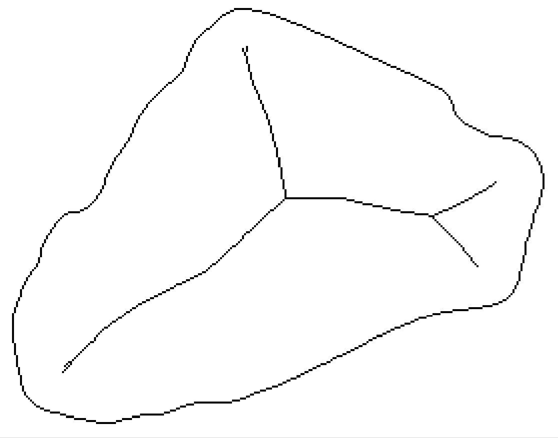
- Clump logic in PFC allows the treatment of element clusters as rigid bodies
- Element density and computation time step were scaled to cluster mass
- Overlapping Discrete Element Cluster technique used for capturing particle shape
- First step in the process is skeletonization, where the skeleton is defined as the locus of centers of maximally inscribed discs or spheres
- Skeletonization process was automated using Matlab™

Particle Shape Modeling in Two Dimensions

Skeletonization



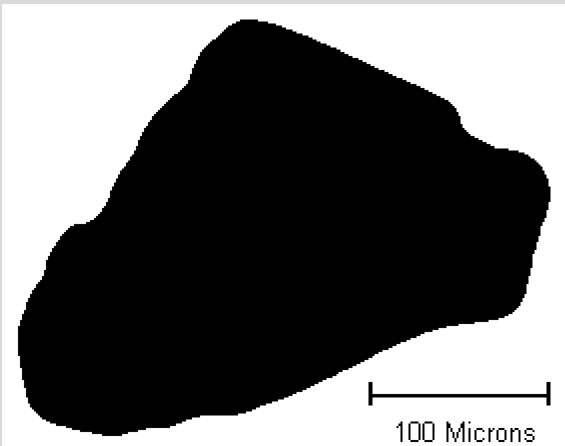
Daytona Beach Sand Grain



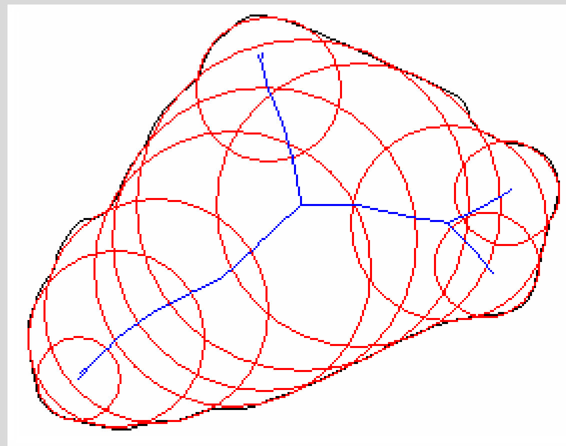
Skeleton

Particle Shape Modeling in Two Dimensions

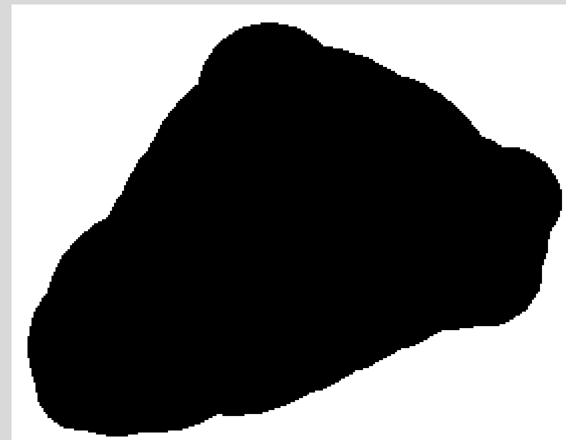
Overlapping Discrete Element Cluster Algorithm: ODEC-2D



Daytona Beach Sand Grain



Skeleton & ODEC

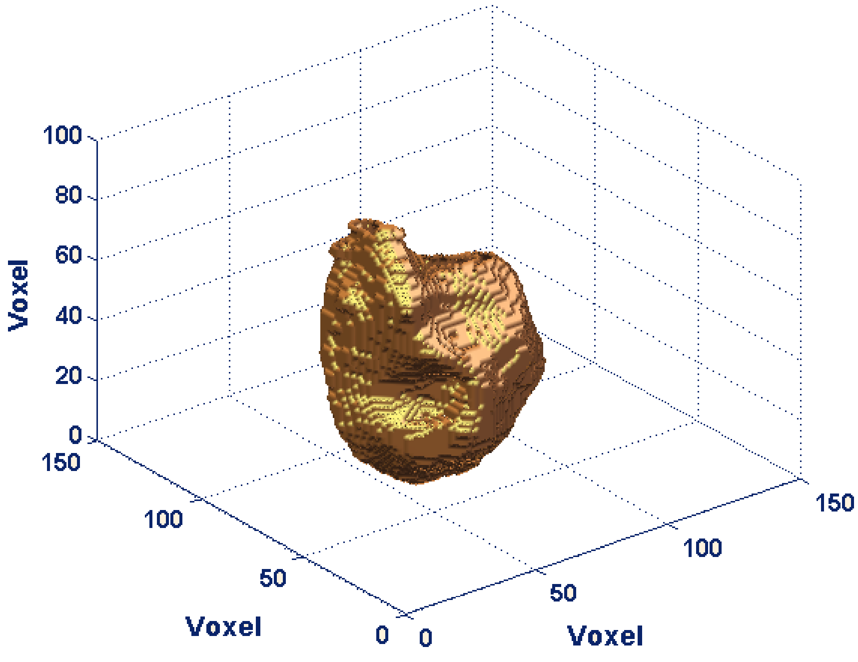


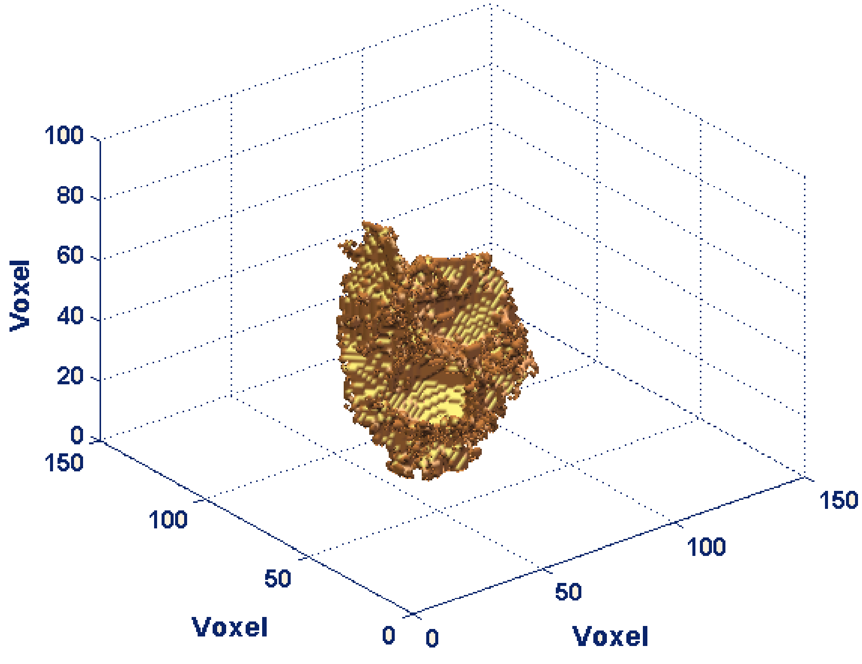
Model Particle

Number of circles needed to capture the shape = 10
Area uncovered < 1%

Particle Shape Modeling in Three Dimensions

Skeletonization



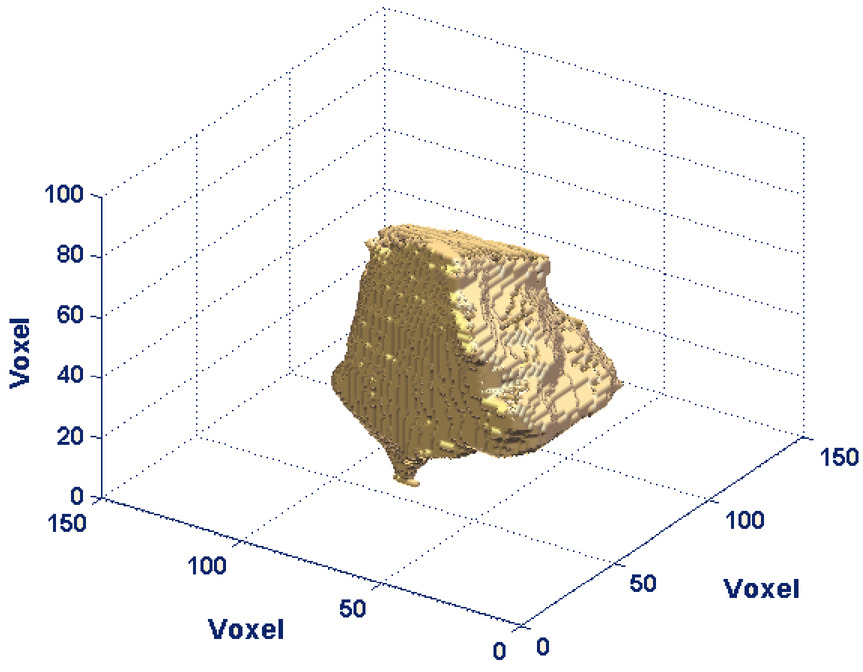


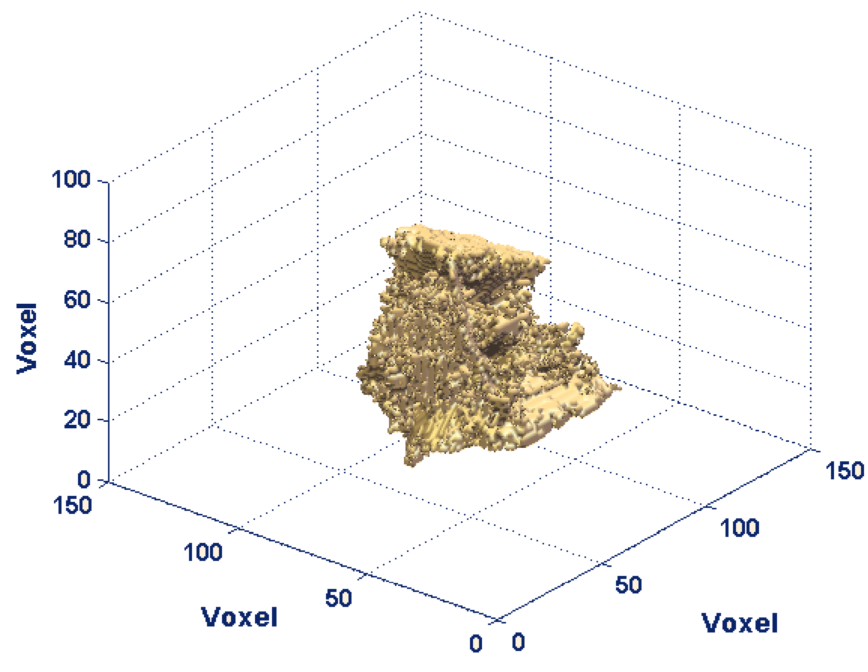
Daytona Beach Sand (Grain 1)

Surface Skeleton

Particle Shape Modeling in Three Dimensions

Skeletonization



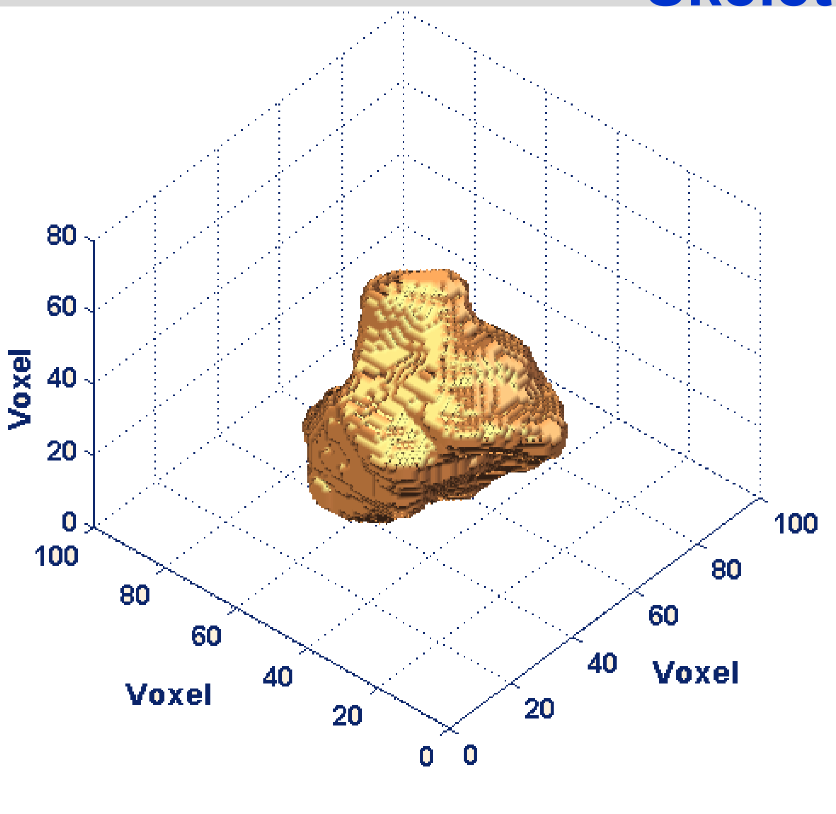


Daytona Beach Sand (Grain 2)

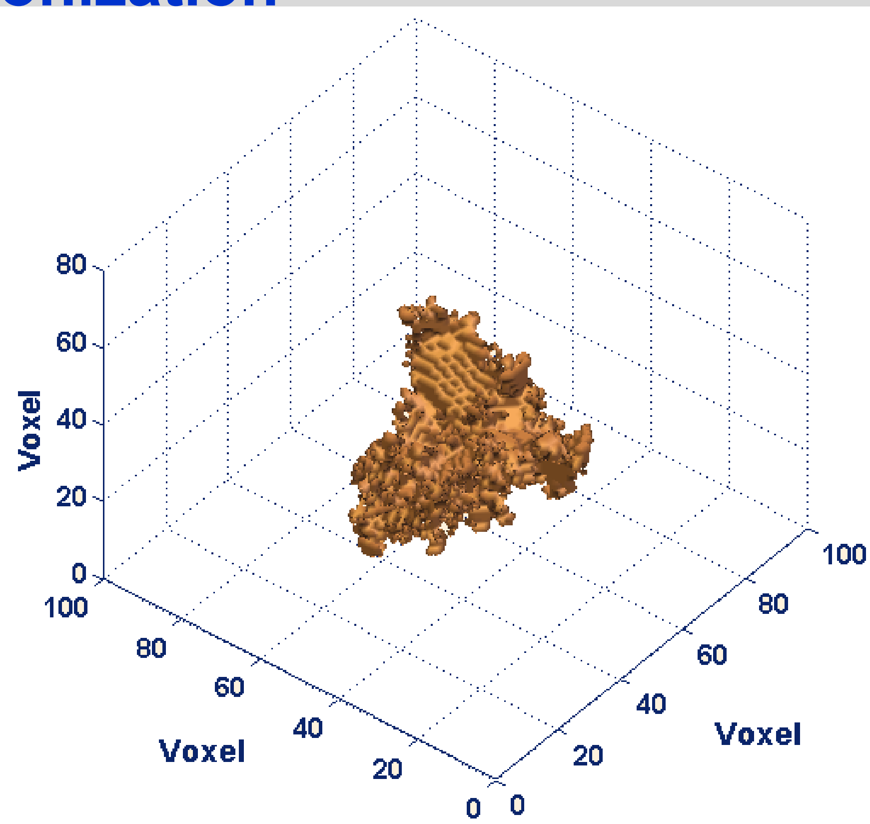
Surface Skeleton

Particle Shape Modeling in Three Dimensions

Skeletonization



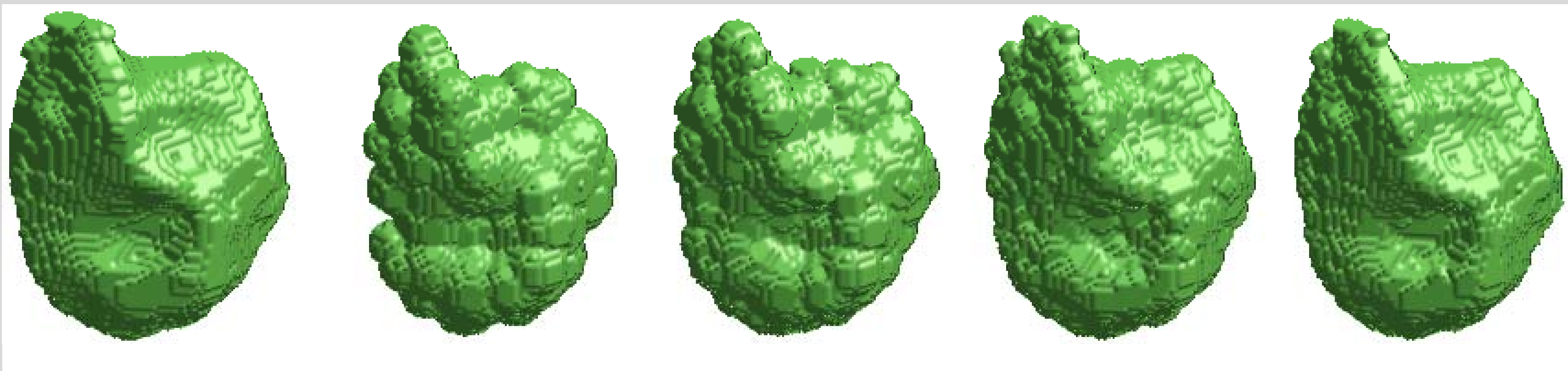
Michigan Dune Sand Grain



Surface Skeleton

Particle Shape Modeling in Three Dimensions

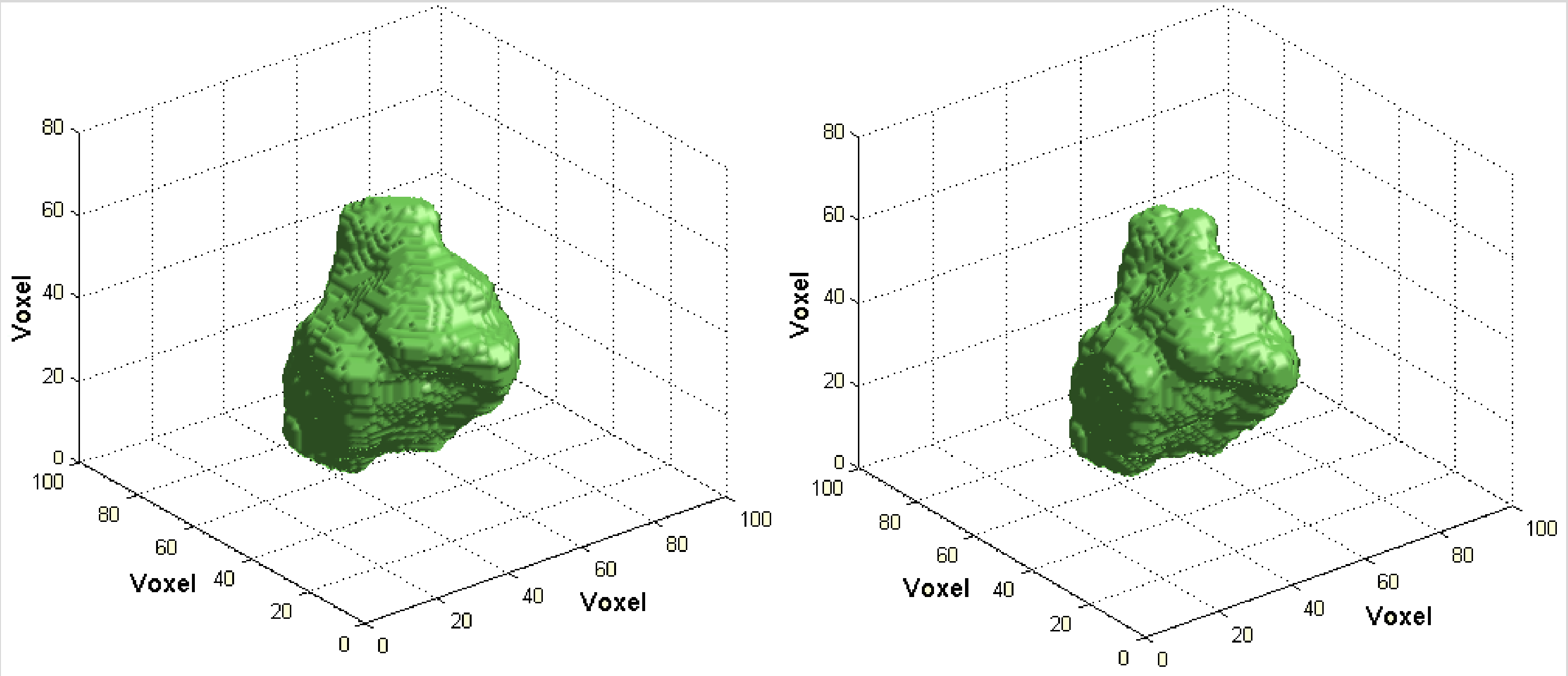
Overlapping Discrete Element Cluster: ODEC-3D



Daytona Beach Sand Grain | 85% Covered | 90% Covered | 95% Covered | 98% Covered

Particle Shape Modeling in Three Dimensions

Overlapping Discrete Element Cluster: ODEC-3D



Michigan Dune Sand Grain **Model Particle**

Number of spheres needed to capture the shape = 98
Volume Covered ≈ 95%

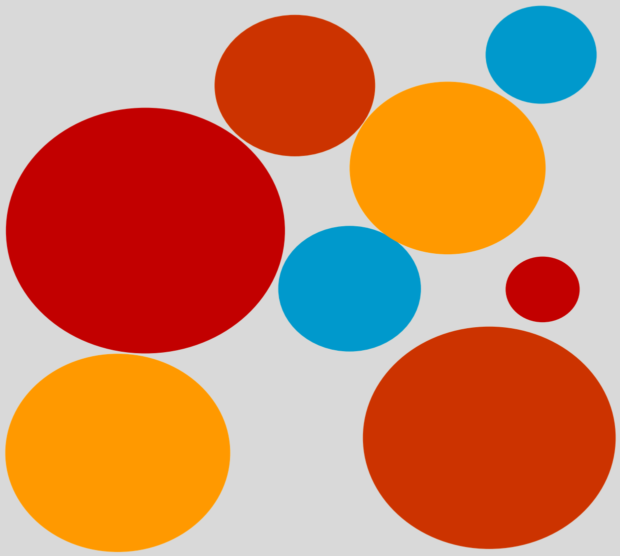
Particle Shape Modeling in Three Dimensions

Volume Covered	Number of Spheres	
	Daytona Beach Sand Sample	Michigan Dune Sand Sample
98%	251 - 296	217 - 297
95%	123 - 133	98 - 126
90%	61 - 62	49 - 57
85%	35 - 39	32 - 34

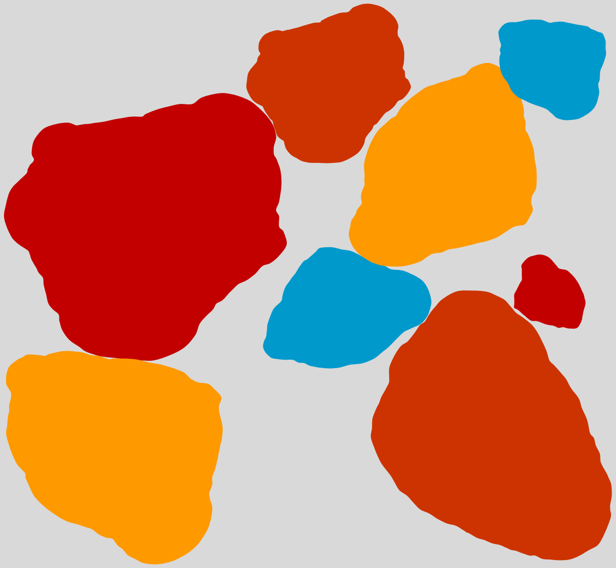
Particle Transformation in PFC code

- Accomplished using FISH subroutines
- Digital particle data are stored in a library of grain shapes
- A unique particle assembly is generated according to a size distribution with circular particles
- Particles are randomly selected from the corresponding shape library for each material and transformed (mapped)
- Mapped particles are rotated to release excessive contact forces due to partial overlapping
- The assembly is subsequently subjected to loading conditions such as isotropic confinement or shear

Particle Transformation



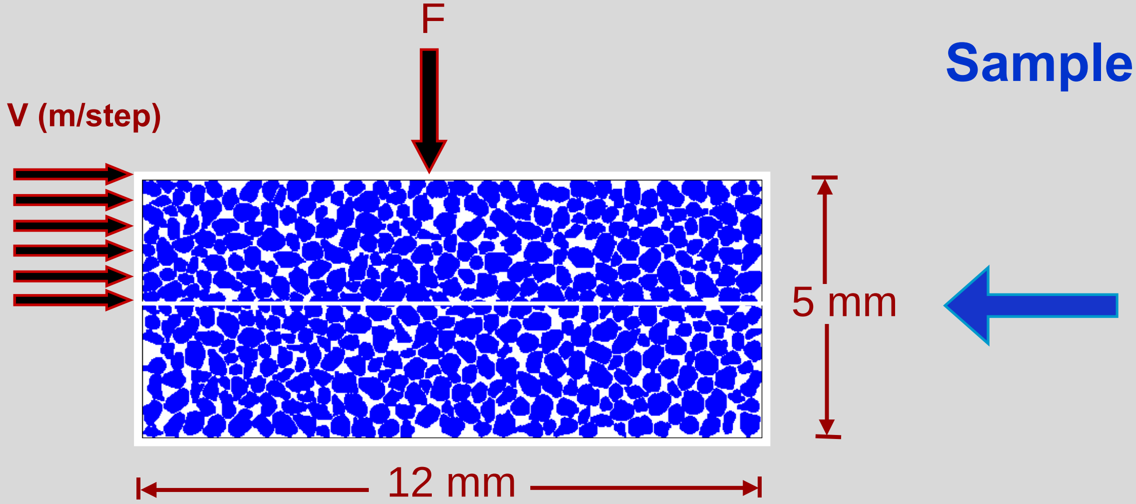
Circular particles generated to a specific grain size distribution



Angular sand equivalent randomly rotated

Results

DEM Simulation of Direct Shear Test in PFC^{2D}



Sample: Daytona Beach Sand

Angular Equivalent of 2-D Circular Particles

Test Parameters

Mean Particle Size = 0.375 mm

Interparticle friction coefficient = 0.5

Porosity = 0.23

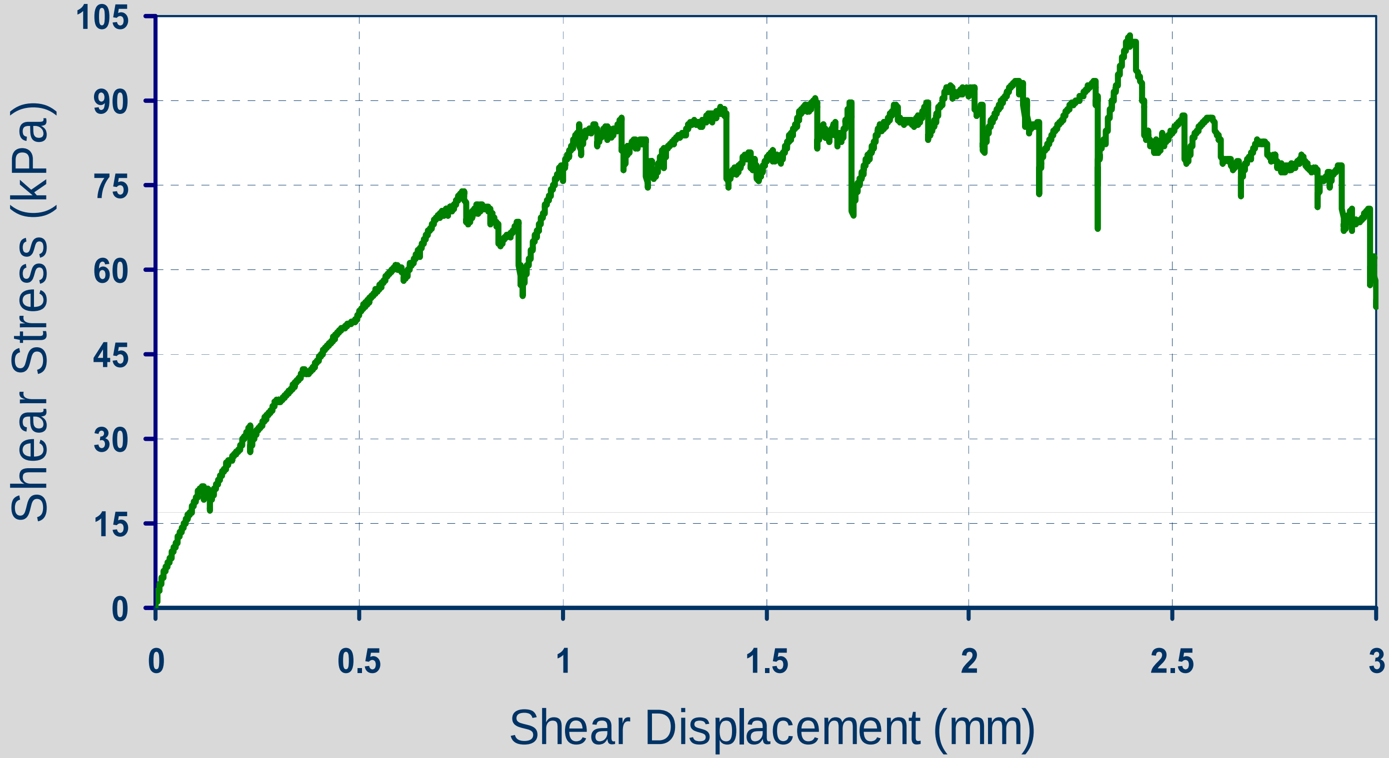
Particle density = 2500 kg/m^3

Velocity, V = 5×10^{-3} m/step

Number of particles = 416

Linear stiffness contact model

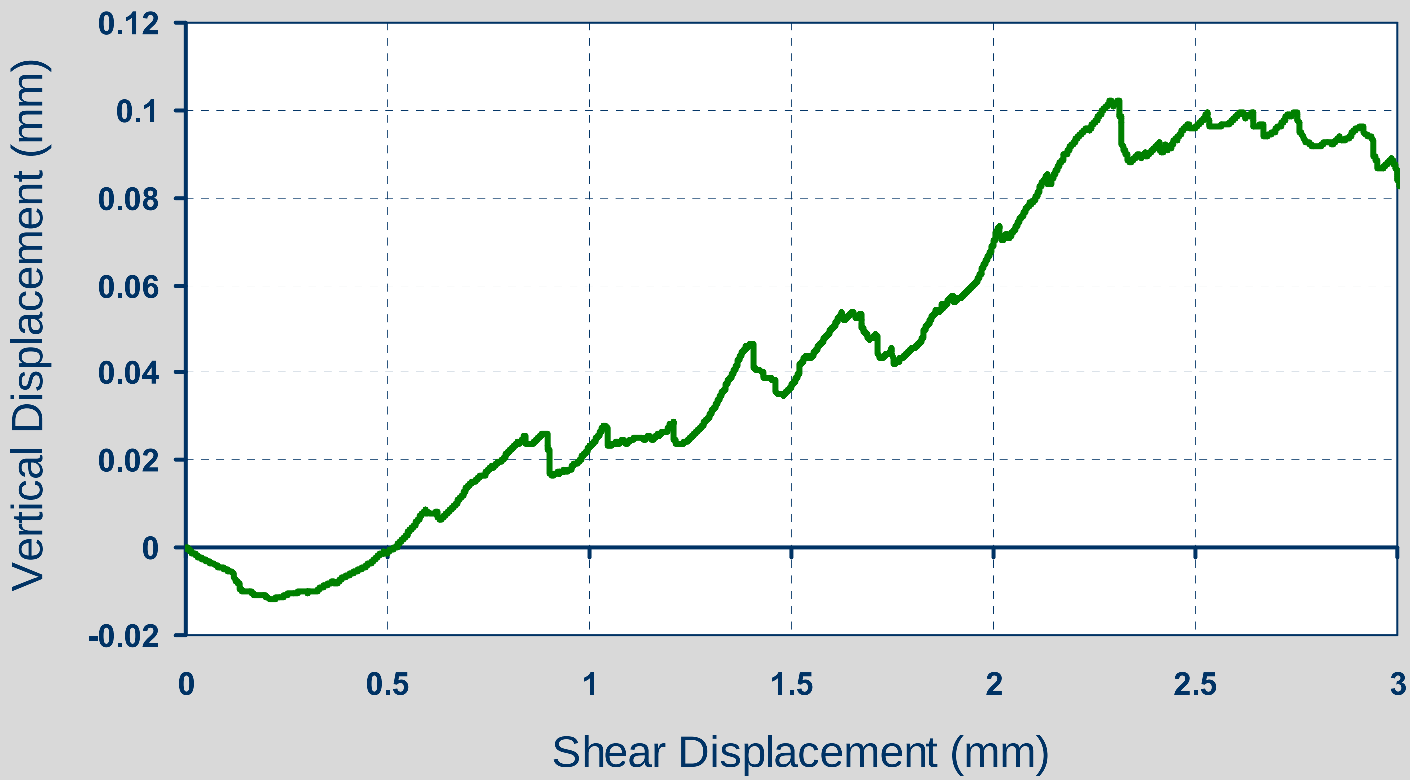
DEM Simulation in Two Dimensions on Daytona Beach sand



Direct Shear Test on Daytona Beach Sand

σ = 200 kPa

DEM Simulation in Two Dimensions on Daytona Beach sand



Direct Shear Test on Daytona Beach Sand

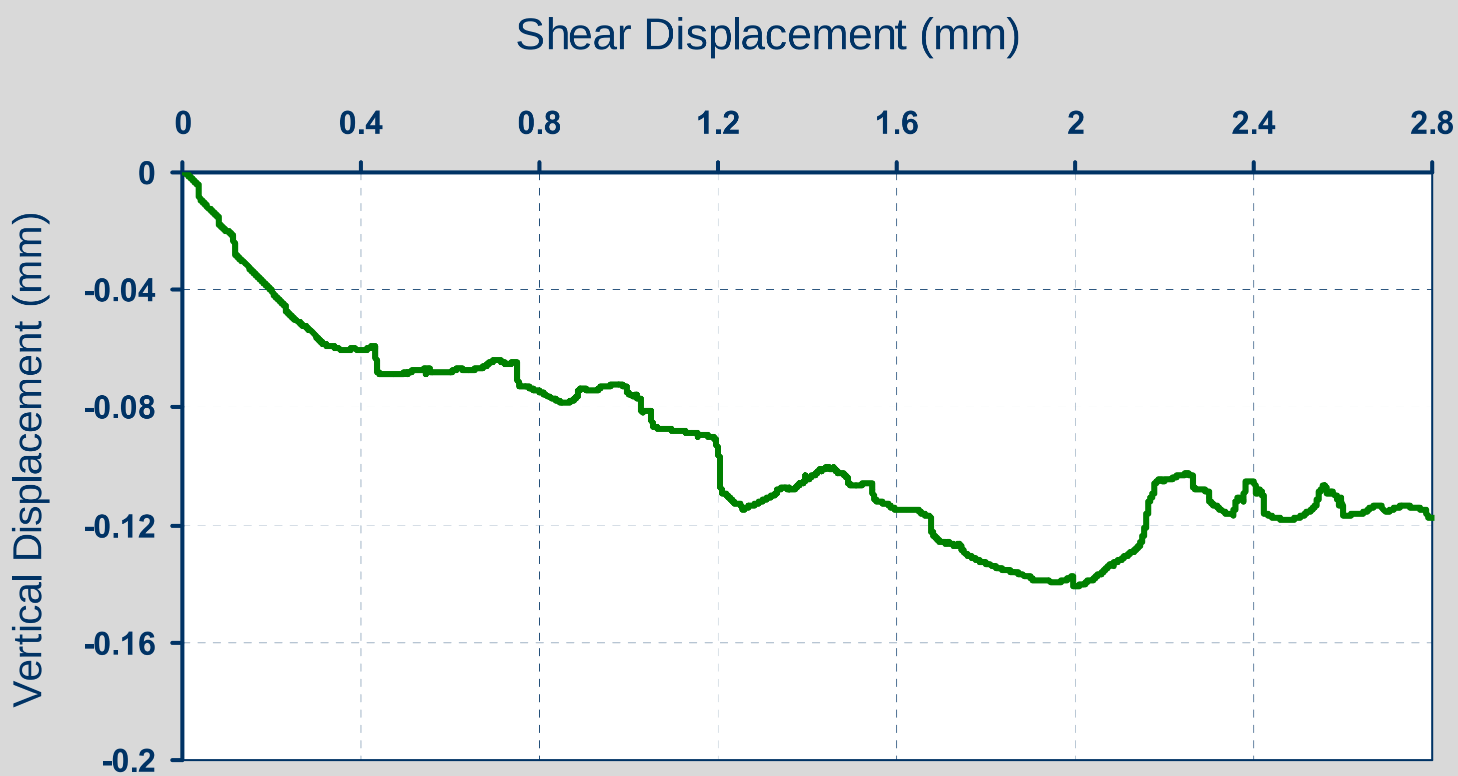
σ = 200 kPa

DEM Simulation in Two Dimensions on Circular Disks

Direct Shear Test on Circular Particles

σ = 200 kPa

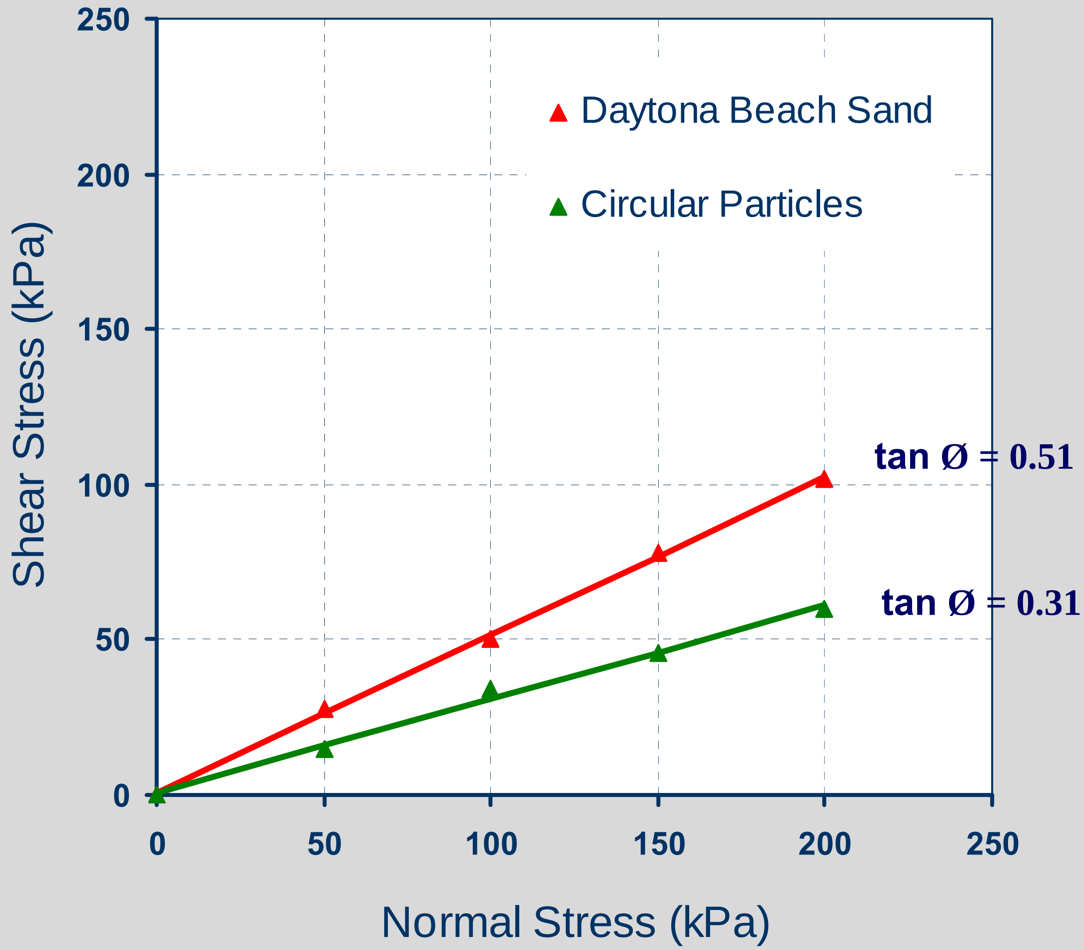
DEM Simulation in Two Dimensions on circular disks



Direct Shear Test on Circular Particles

σ = 200 kPa

DEM Simulation in Two Dimensions



DEM Simulation of Direct Shear Test in PFC^{3D}

Test Parameters

Mean Particle Size = 0.375 mm

Interparticle friction coefficient = 0.5

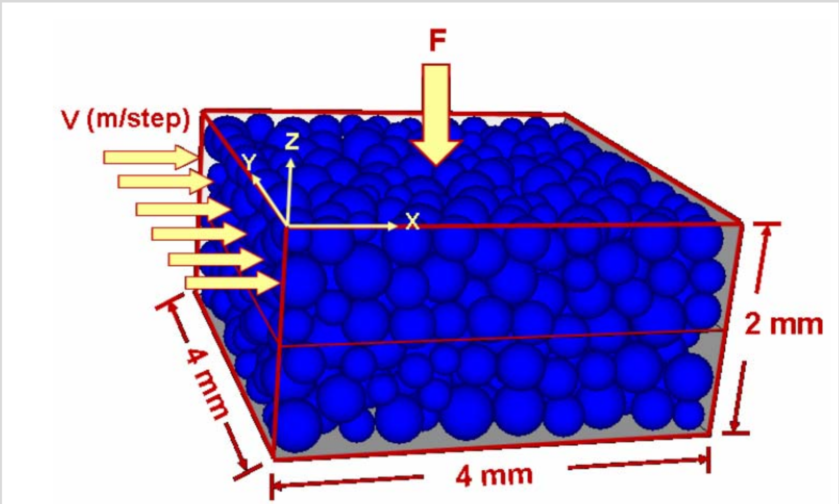
Porosity = 0.30

Particle density = 2500 kg/m^3

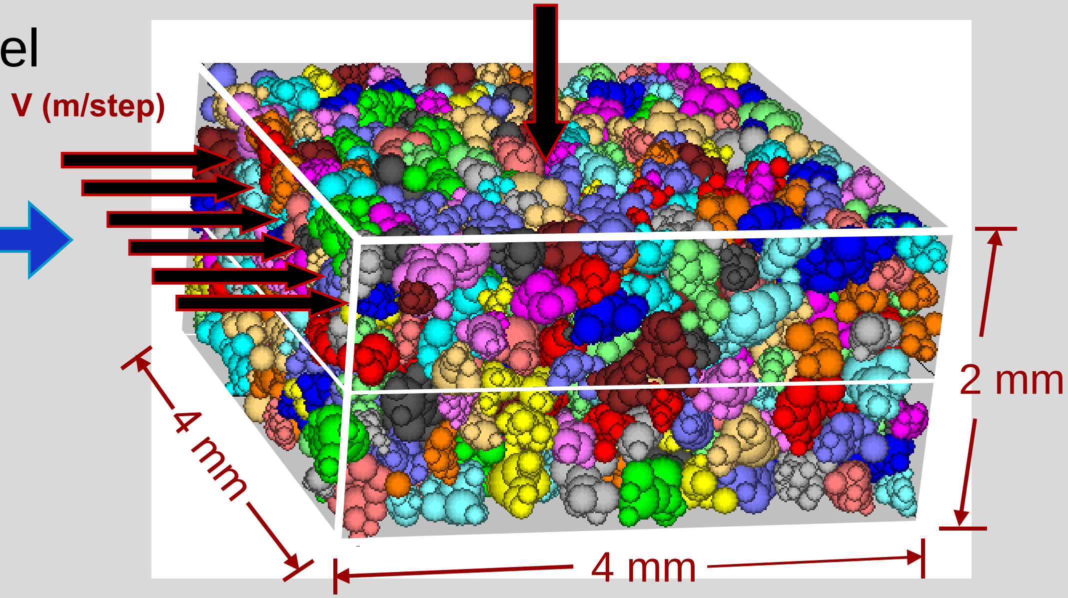
Number of particles = 800

Velocity, V = 5×10^{-3} m/step

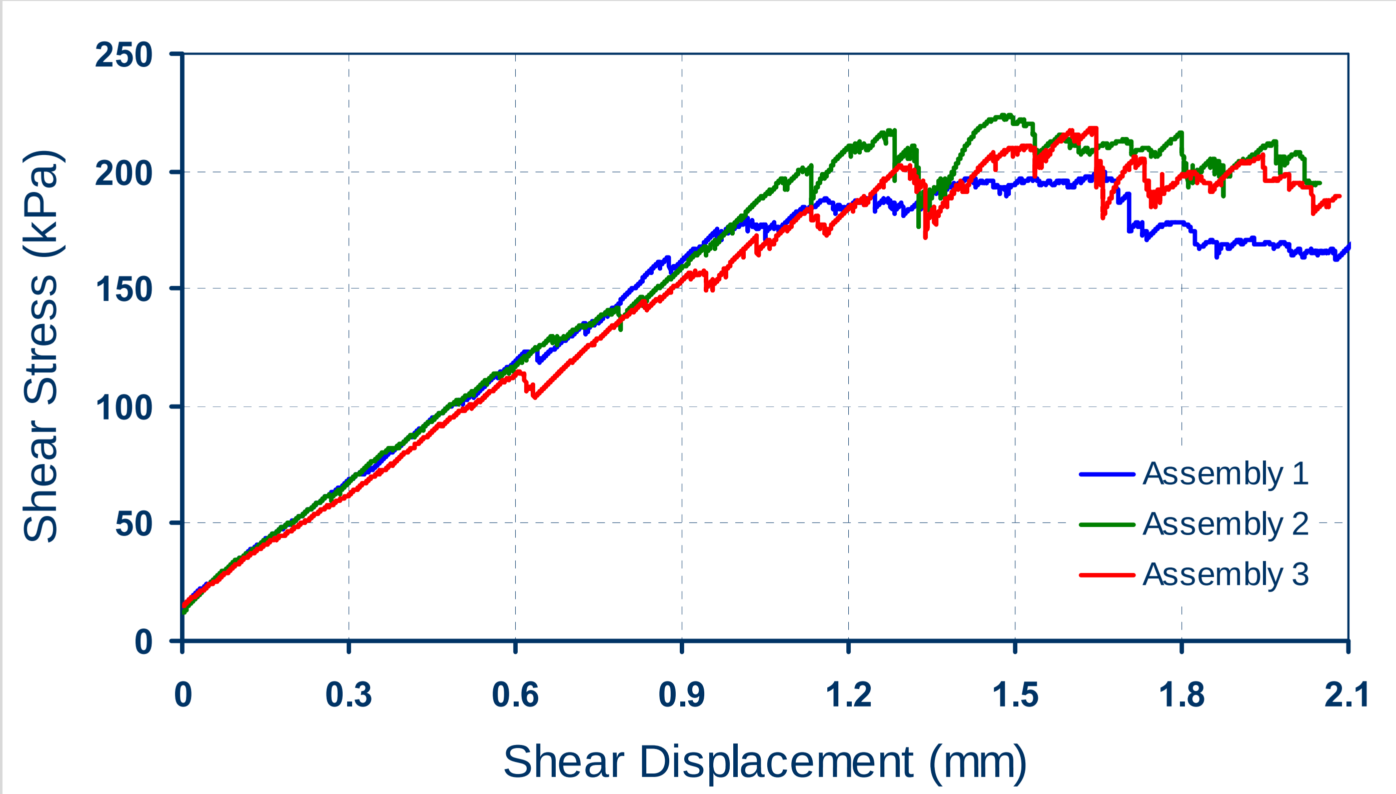
Linear stiffness contact model



Angular Equivalent of 3-D Spherical Particles



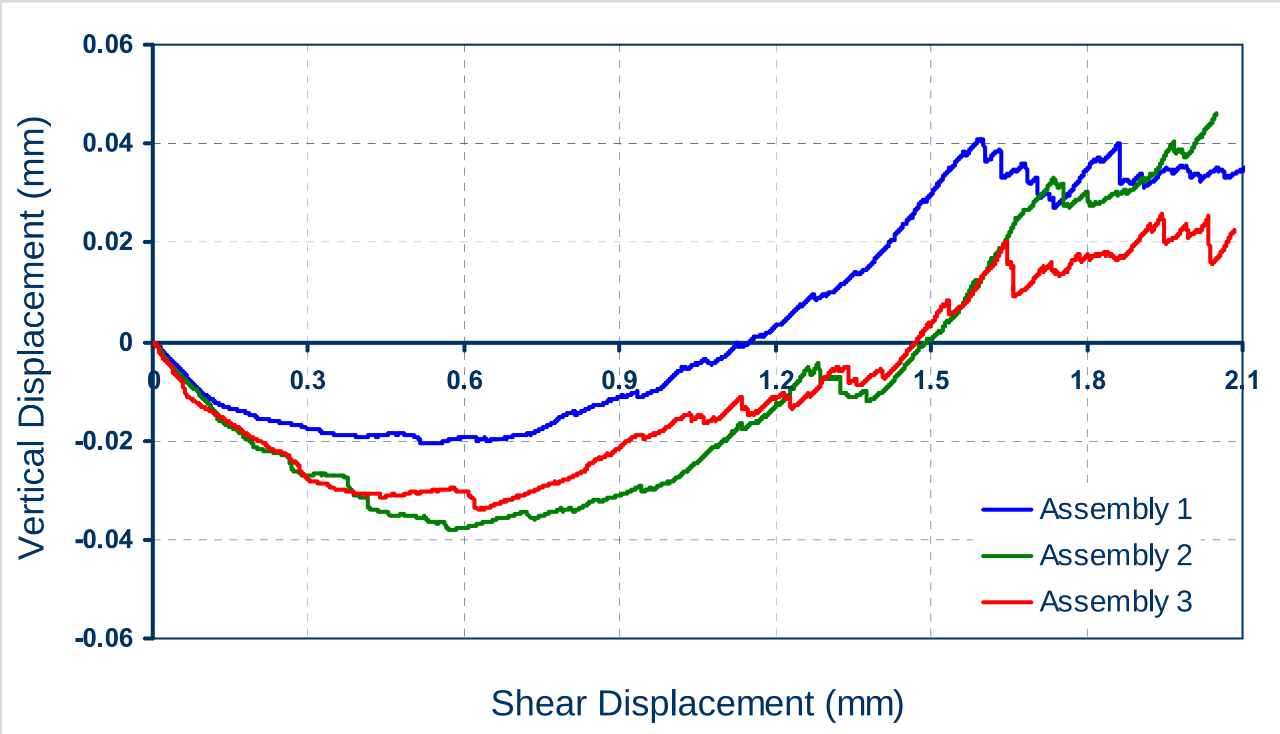
DEM Simulation in Three Dimensions on Daytona Beach sand



Direct Shear Test on Daytona Beach Sand

(σ = 250 kPa)

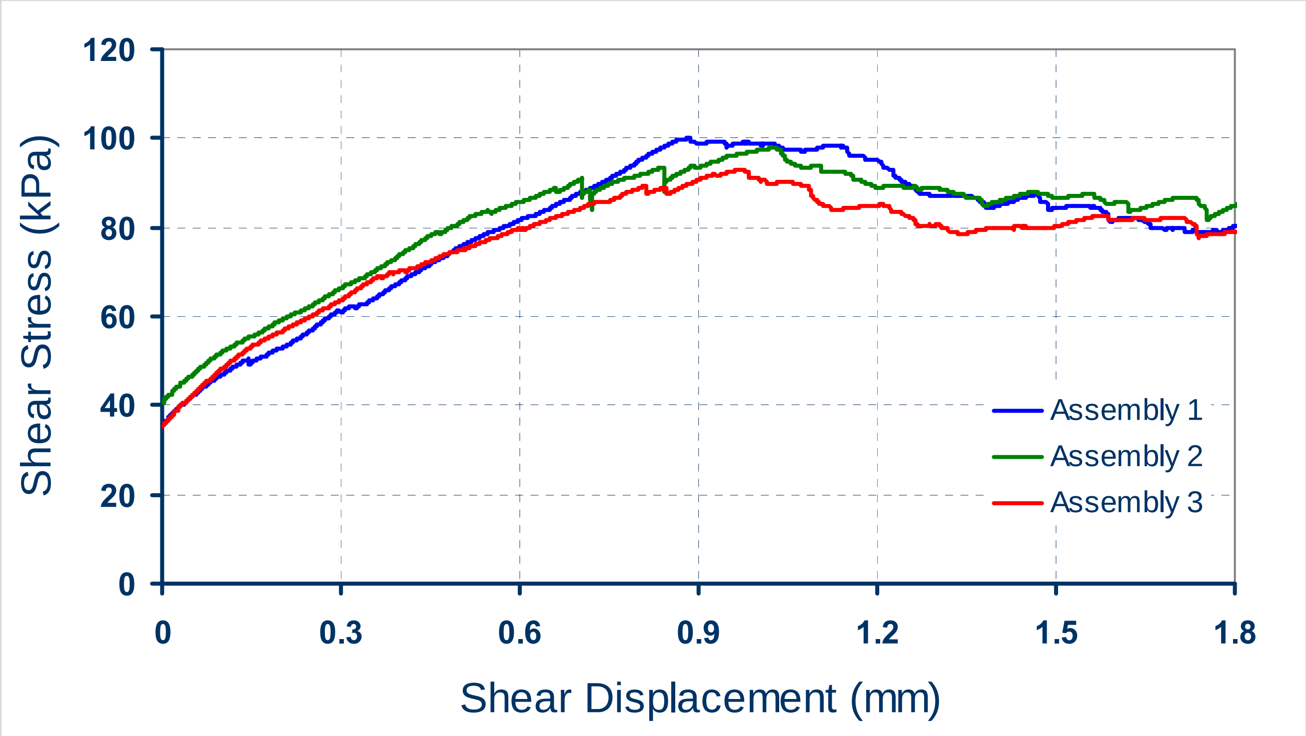
DEM Simulation in Three Dimensions on Daytona Beach sand



Direct Shear Test on Daytona Beach Sand

(σ = 250 kPa)

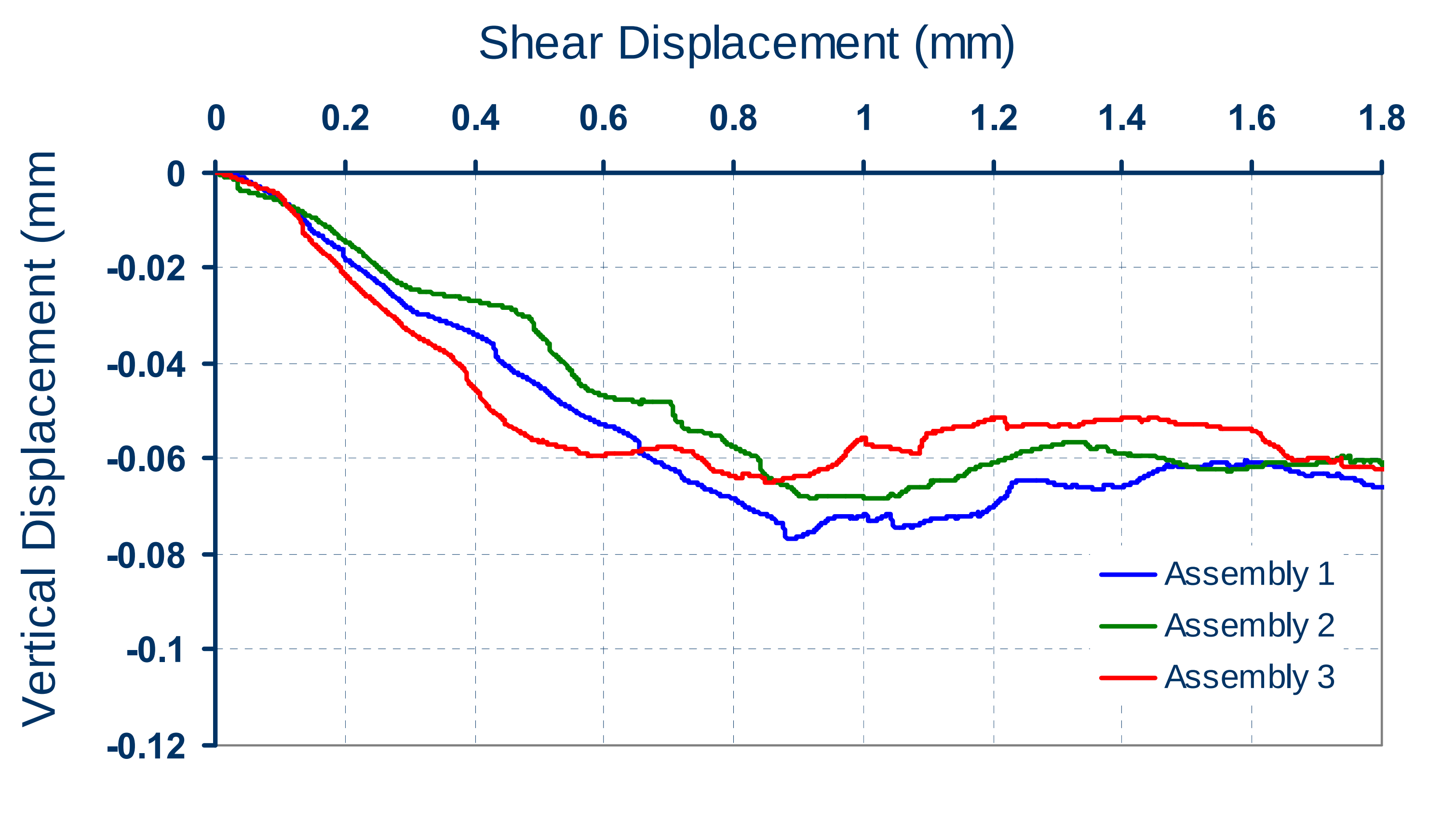
DEM Simulation in Three Dimensions on spherical particles



Direct Shear Test on Spherical Particles

(σ = 200 kPa)

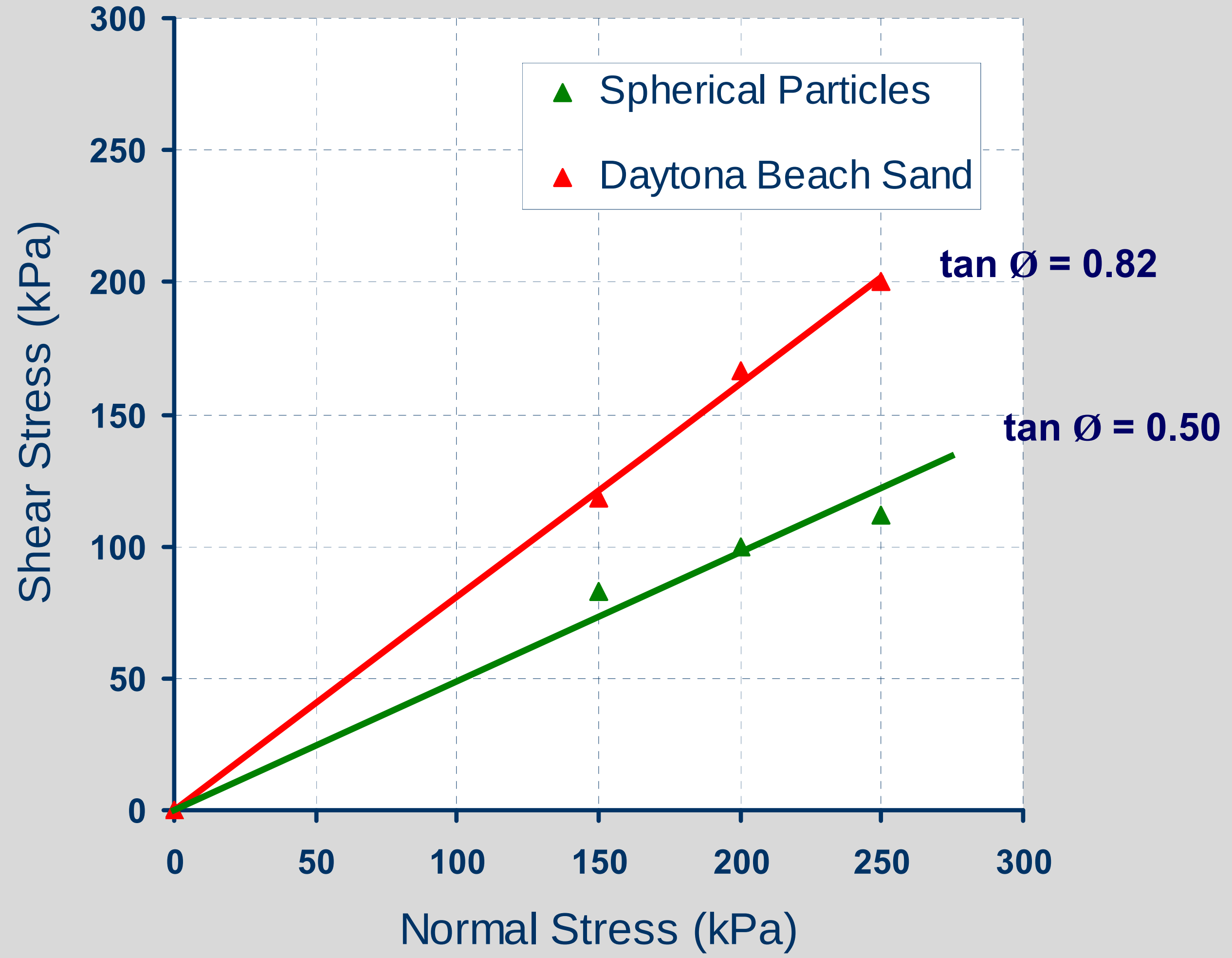
DEM Simulation in Three Dimensions on spherical particles



Direct Shear Test on Spherical Particles

(σ = 200 kPa)

DEM Simulation in Three Dimensions



DEM Simulation in Three Dimensions

Angle of Internal Friction from 2-D and 3-D Simulation

Material	2-D Simulation	3-D Simulation	Experimental values
Daytona Beach Sand	27°	39° – 43°	37.4°
Rounded Particles	17.2°	25° - 26.6°	24.4° – 27° *

* O'Sullivan et al. (2004); Phillips et al. (2006)

Conclusions

- ODEC2D and ODEC3D algorithms can model irregular 2-D and 3-D particle shape with desired accuracy
- Stress-strain and volumetric behavior of simulated material followed typical soil behavior of angular and rounded particles
- The angles of shearing resistance obtained using three different fabrics in 3-D simulation are very close to each other for both Daytona beach sand and rounded spheres
- Angularity and particles interlocking resulted in more shearing resistance in Daytona Beach sand compared to rounded material

Acknowledgments

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